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MCNPX, VERSION 2.6.B

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ABSTRACT

MCNPX is a Fortran90 Monte Carlo radiation transport computer code that transports nearly all particles at nearly all energies for nearly all applications. The new capabilities of the latest version, MCNPX 2.6.B, are described.

1.0. INTRODUCTION

MCNPX (MCNP eXtended) is a Fortran90 (F90) Monte Carlo radiation transport computer code that transports nearly all particles at nearly all energies. It is a superset of MCNP4C3 and has many capabilities beyond MCNP4C3. MCNPX is a production computer code that models the interaction of radiation with matter, and its quality is guaranteed; it can be used with confidence. The MCNPX guarantee is described in Section 1.1.4.

1.1. Summary of New MCNPX Features

The new capabilities and enhancements of MCNPX 2.6.B beyond MCNPX 2.5.0 are listed as follows (where applicable, the initials of the principal developers are shown in parentheses):[1]

- depletion/burnup,[2]
- CEM03 physics,[3]
- corrections/enhancements/extensions
    - new photon emission data: PHTLIB (REP/GWM),
    - geometry plot basis vectors (GWM),
    - extend ZAID identifiers (GWM),
    - LINLIN contour plot defaults (GWM), and
    - additional enhancements and corrections.

MCNPX 2.6.B also includes the following MCNPX 2.6.A capabilities:

- depletion/burnup,
- long file names (JSH),

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[1] John S. Hendricks (JSH, LANL, D-5); Gregg W. McKinney (GWM, LANL, D-5). Robert E. MacFarlane (REM, LANL, T-16),

[2] The depletion/burnup capability is based on CINDER 90, which was written by William B. Wilson (LANL, T-16), and MonteBurns, which was written by Holly R. Trellue (LANL, X-1). The initial patch to MCNPX was developed by GWM and Joe W. Durkee (JWD, LANL, D-5). MCNPX26a and MCNPX 26b were written mainly by Michael L. Fensin (MLF, D-5).

[3] CEM03 was developed mostly by Stepan G. Mashnik (LANL, X-3), with algorithms developed by Arnold J. Sierk (LANL, T-16). LAHET was written by Richard E. Prael (REP, LANL, X-3) and adapted into MCNPX 26B by GWM.

- tallies terminated at desired precision: STOP card (JSH), and
- corrections/enhancements/extensions
  - proton step size control: HSTEP on M card (GWM),
  - new S(α,β) scattering law (REM/GWM/JSH),
  - differential data tallies extended to table physics (GWM),
  - separate printout of induced fission multiplicity (JSH),
  - removal of tracking fixes (JSH), and
  - additional enhancements and corrections.

1.2. Availability

The latest general-release version of MCNPX is MCNPX 2.5.0, which is available from the Radiation Safety Information and Computational Center (RSICC)[1] and the Office of Economic Cooperation and Development/Nuclear Energy Agency (OECD/NEA) in Paris, France.[2]

For approved users, beta test program versions, including MCNPX2.6.B, may be downloaded from the MCNPX website.[3] Approximately 1600 MCNPX beta test users are an essential part of the MCNPX software quality assurance program. To become a new beta test user usually requires being an MCNPX sponsor, collaborator, or participant in an MCNPX workshop training course. For more information, contact mcnpx@lanl.gov.

MCNPX is US export controlled. Generally, MCNPX is easy to obtain for legitimate purposes, but restrictions protect the code, data, and documentation once it is acquired.

1.3. Documentation

Restricted Documentation:

Complete MCNPX documentation is available in the "MCNPX User's Manual,"[4] which comes with MCNPX from RSICC and is available to MCNPX beta testers from the Worldwide Web (WWW).[5]

Unrestricted Documentation:

Documentation of MCNPX features in MCNPX 2.5.0—that is, all MCNPX features beyond MCNPX2.3.0 and MCNP4C—is provided in "MCNPX Extensions, Version 2.5.0."[6]

MCNPX capabilities developed since the RSICC's international release version, MCNPX 2.5.0 (namely, the capabilities of MCNPX 26a and MCNPX 26b), are documented herein.

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1 http://www-rsicc.ornl.gov/.
2 http://www.nea.fr/.
3 http://mcnpx.lanl.gov/beta/.
4 http://mcnpx.lanl.gov/docs/MCNPX_2.5.0_Manual.pdf/.
5 http://mcnpx.lanl.gov/.
6 http://mcnpx.lanl.gov/opendocs/reports/Interface.pdf/.

All of the extended MCNPX capabilities are summarized in the one-page MCNPX features list.[1]

1.4. Guarantee

MCNPX is guaranteed. We are so confident of the quality of MCNPX that we will pay $20 to the first person finding anything that does not meet or exceed the capabilities of MCNPX 2.3.0 and MCNP4C3. European users will be awarded €20. We also will pay a brand new $2 bill for any error in MCNPX that has been inherited from its constituent codes.[2] A list of all winners since June 2001 can be found on the MCNPX WWW site.[3]

2.0. DESCRIPTION OF NEW MCNPX FEATURES

The principal new capabilities of MCNPX beyond MCNPX 2.5.0 are

- depletion/burnup,
- CEM03 physics,
- long file names, and
- tallies terminated at desired precision: STOP card.

2.1. Depletion/Burnup

The depletion/burnup capability is based on CINDER 90, which was written by William B. Wilson (LANL, T-16), and MonteBurns, which was written by Holly R. Trellue (LANL, X-1). The initial patch to MCNPX was developed by Joe W. Durkee and Gregg W. McKinney. Most of the corrections and enhancements to MCNPX 26A and 26B were developed by Michael L. Fensin (LANL, D-5) and integrated by John S. Hendricks (LANL, D-5).[4,5] Currently, the depletion/burnup/transmutation capability is limited to criticality (KCODE) problems.

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[1] http://mcnpx.lanl.gov/opendocs/misc/FeaturesList.pdf/

[2] Cash Award Fine Print: This offer is subject to cancellation or modification without notice. A bug is defined as an error we choose to correct in the source code. We make awards even for the most trivial or insignificant of problems, but not for proposed code enhancements or proposed extended capabilities. Awards are given only to the first MCNPX user reporting a problem. Reported problems must be reproducible, and awards are paid when the correction is integrated into a forthcoming MCNPX version. We endeavor to make MCNPX the most error-free and robust Monte Carlo radiation transport code possible, and we back this code with a cash guarantee.

[3] http://mcnpx.lanl.gov/opendocs/misc/Cashbugs.pdf/.

[4] Michael L. Fensin, John S. Hendricks, and Samim Anghaie, "Enhanced Monte Carlo Linked Depletion Capabilities in MCNPX" (Abstract: Los Alamos National Laboratory report LA-UR-05-9559) 2006 International Congress on Advances in Nuclear Power Plants Embedded International Topical Meeting at the 2006 ANS Annual Meeting, ICAPP '06, Reno, Nevada (June 4–8, 2006).

[5] Michael L. Fensin, John S. Hendricks, Gregg W. McKinney, and Holly Trellue, "Advances in Monte Carlo Depletion Capabilities for MCNPX," Los Alamos National Laboratory report; abstract: LA-UR-05-7895, full paper: LA-UR-06-0629. American Nuclear Society 14th Biennial Topical Meeting of the Radiation Protection and Shielding Division, Carlsbad, New Mexico (April 3–6, 2006).

The new MCNPX 26B capabilities are

- "MONTEBURNS" predictor corrector methodology;
- automatic fission yield selection;
- 1-group reaction rate reporting;
- corrected power fraction/individual burn material burnup calculation;
- multiprocessor (MPI) capability;
- defaults for most of the burn card flags:
    - If pfrac not selected, *PFRAC* = 1 for each burn step;
    - If burn materials not selected, then burn all materials.
- fatal-error message if cinder.dat library cannot be found.

2.1.1. Depletion Process

MCNPX depletion is a linked process involving steady-state flux calculations in MCNPX and nuclide depletion calculations in CINDER90. MCNPX runs a steady-state calculation to determine the system eigenvalue, 63-group fluxes, fission rates, absorption rates, ν, and Q values. CINDER90 then takes those MCNPX-generated values and carries out the depletion calculation to generate new number densities at the following time step. MCNPX then takes those new number densities and generates another set of fluxes and reaction rates; the process repeats itself until after the final time step.

MCNPX calculates parameters only for those materials listed on the MCNPX material cards, produced by the isotope generator algorithm, or selected by the specified fission product tier. However, CINDER90 tracks the time-dependent reactions of 3456 isotopes using intrinsic cross-section and decay data inherent in the CINDER90 code when the information is not specified from MCNPX. Although MCNPX tracks only certain specified isotopes that contain transport information, CINDER90 continues to track the data of all 3456 isotopes using nuclide densities from the prior time step to do the burnup calculation for the following time step. Therefore, even though an isotope in a certain decay chain may not be listed in an MCNPX calculation, the full decay process still is tracked in the CINDER90 code exactly; therefore, the isotope concentrations reported are still true isotope concentrations.

For MCNPX to burn materials properly, the user must point to the CINDER.dat library file. This file contains decay, fission yield, and 63-group cross-section data not calculated by MCNPX. The CINDER.dat library file will be accessed properly by the code if the file is placed in the working directory in which the user is executing MCNPX or in a directory in which the command window PATH is set to the command window. If the code cannot find the CINDER.dat, a fatal-error message will be printed and the case will cease calculation.

2.1.2. Collision Density Generation

MCNPX calculates continuous energy reaction rates for (n,gamma), (n,f), (n,2n), (n,3n), (n,alpha) and (n,proton). CINDER90 must use the MCNPX-calculated 63-group fluxes to determine the rest of the interaction rates that accumulate in the transmutation process.

The collapsed 1-group reaction rates calculated in MCNPX for use in the CINDER90 code for depletion are printed at the end of each kcode cycle. Reaction rates are printed only for those isotopes also used in the transport calculation.

For example, MCNPX currently does not calculate the continuous (n, beta) reaction rates. CINDER90 must take the 63-group flux calculated by MCNPX and multiply its inherent 63-group (n, beta) cross section to determine the amount of (n,beta) reactions in the system. The 63-group cross sections in CINDER90 were collapsed over a generic spectrum that may or may not be representative of the system to be analyzed and thus may lead to large discrepancies in the isotope inventory of daughter products from these reactions.

2.1.3. The Predictor Corrector Methodology

The depletion equations use fluxes, nuclide number densities, and cross sections to determine the time-dependent nuclide inventory. The simplified one-group depletion equation is

$$\frac{dN(r,t)}{dt} = -\Phi(r,t) * \sigma(r) * N(r,t) \quad .$$

The corresponding solution for nuclide density is

$$N(r,t) = N_0(r)e^{-\sigma(r)\int_{t_1}^{t_2}\Phi(r,t)dt} \quad .$$

Therefore, the change in nuclide concentration is dependent on the time-integrated flux. Unfortunately, the time-dependent flux (integrated to get the time-integrated flux) also is dependent on the nuclide density, which makes the above equation circular and unsolvable. To make the above equation solvable, an assumption must be made about the time-dependent flux. MCNPX currently assumes that the flux is constant throughout the burn step:

$$N(r,t) = N_0(r)e^{-\sigma(r)\Phi(r)_{t,average}} \quad .$$

This approximation is true only if the average flux used in the calculation is the "true average" flux over the burn step.

MCNPX makes an approximation of the average flux behavior by using a predictor corrector technique. This technique implemented in MCNPX involves the following multistep process:

1. A burnup calculation is completed in CINDER90 to the half time step [t(1)→t(1+1/2)] (Predictor Step).

2. Fluxes and collision densities are recalculated in a steady-state MCNPX calculation at the half-time step.

3. The recalculated fluxes and collision densities then are used to burn over the full time step [t(1)→t(2)] (Corrector Step).

The fluxes and collision densities recalculated at the half time step are assumed to be the average fluxes and collision densities encountered during the entire time step. This approximation is true only if the flux shape change between the two time steps varies linearly; in most cases, this technique is usually an acceptable approximation. Implementing this technique allows the user to burn a system using fewer burn steps than if no approximation were made on the average flux behavior.

However, even with this approximation, burning with large time steps that encounter large flux-shape changes during the time step will lead to inaccurate calculations. Therefore, the user must use time steps that are small enough to capture the flux-shape change accurately over time.

2.1.4. BURN Card Setup

The following example explains the setup for a BURN card.

```
BURN    TIME=T1,T2,T3,...
        PFRAC=F1,F2,F3,...
        POWER=P
        MAT=M1,M2,M3,...
        OMIT=J1,N1,I11,I12,...,J2,N2,I21,I22,...
        AFMIN=A
        BOPT=B1,B2,B3   ,
```

where

Ti = duration of burn step i (days). Default is one time step of one day.

Fi = power fraction of each time step (0–1). The default for this parameter is to assume Fi = 1.0 for each time step if a *PFRAC* flag is not specified at all.

P = power level (MW). Default is 1.0 MW.

Mi = list of material numbers to include in the burn. The default for this parameter is to burn all materials.

Ji = ith material for which to omit nuclides Ii1, Ii2, etc. Currently, there is no default for this parameter.

Ni = number of omitted nuclides listed for the ith material. Currently, there is no default for this parameter.

Ii1, Ii2, ... = 1st, 2nd, etc. omitted nuclides for the ith material. Currently, there is no default for this parameter.

A = atom fraction minimum below which the atom fraction is set to zero. Default is 1.0e-10.

B1 = Q value multiplier. Default is 1.0.

B2 = burn table output frequency, ordering, and content flag.

Input Value	Output Inventory Ordering
1 (default)	High to low, based on mass
2	High to low, based on activity
3	High to low, based on specific activity
4	Increasing zaid

Positive input values cause output to be printed only at the end of the entire job. Negative input values cause output to be printed at the end of each burn step. Three tiers of fission-product content are available. To specify the content, add zero (default), 10, or 20 to the magnitude of the B2 Input Value.

TIER	Fission-product content.
1 (default)	Zr-93,Mo-95,Tc-99m,Ru-101,Xe-131,Xe-134, Cs-133,Cs-137,Ba-138,Pr-141,Nd-143,Nd-145.
2	All incident neutron cross sections contained in the Fp array included in the current (v250) XSDIR.
3	All isotopes contained in the Fp array.

B3 = Models option

-1	Fatal error if models are used in the problem.
0	Zeros out the atom fraction of any data using a model. This option runs only if the number of isotopes needed to be zeroed out does not exceed 100. It is preferable to determine which isotopes are needed to be zeroed out and place them on the omit card for the burned material; however, this option exists as a simpler alternative to the omit card.
1	Runs with models.

A blank BURN card will run a case for 1 day, at 1 MW, with a corresponding *PFRAC* = 1.0, burning all materials, using the TIER 1 fission products, and listing the nuclide output in high-to-low mass (as long as the isotope generator algorithm does not generate a nuclide in which there exists no transport cross sections in the XSDIR, which ultimately would lead to a fatal error).

2.1.5. Burn Time, Total System Power, and Power Fraction

The *TIME* flag corresponds to the incremental time duration for each depletion step. Each "Ti" listed in this flag corresponds to a time duration (days) in which the system is burned.

For example:

TIME = 10, 100, 15 .

The system is first burned for 10 days, followed by a 100-day burn, followed by a 15-day burn, for a total burn of 125 days.

The *POWER* flag is the total system power level (in megawatts). Because this value corresponds to the total prompt recoverable energy from the system, the value entered on this flag should correspond to the total prompt recoverable thermal system power.

For example:

POWER = 100 .

In this case, the total recoverable thermal system power is assumed to be 100 MW.

MCNPX depletion accounts only for prompt recoverable energy from the fission process and does not consider those delayed reactions that lead to a decrease in recoverable energy (mentioned later in this section); therefore, this value may need to be adjusted appropriately for proper depletion.

The *PFRAC* flag corresponds to the fractional value of total system power (*POWER*) in which to burn the system for the equivalent time duration. This flag was implemented to account for power level changes occurring during system life as a result of the startup process or the need to down-power the system for system maintenance. For each Ti value listed on the *TIME* flag, a corresponding Fi value listed on the *PFRAC* flag must exist.

For example:

TIME = 11, 33, 22 ,
PFRAC = 1.0, 0.9, 1.2 , and
POWER = 10 .

For the first 11 days of system life, the system is burned at 1.0*10 MWth of the total system power at 10 MWth. For the next 33 days of system life, the system is burned at 0.9*10 MWth of the total system power at 9 MWth. For the final 22 days of system life, the system is burned at 1.2*10 MWth of total system power at 12 MWth.

2.1.6. Flux Normalization Parameters

MCNPX generates collision densities for the CINDER90 depletion calculation. These generated collision densities are normalized per source neutron. CINDER90 requires a total flux to deplete the system appropriately. The following flux multiplier is calculated to transform the MCNPX normalized flux into a total flux for the CINDER90 depletion calculation:

$$\phi_{total} = \phi_{MCNPX} \times Flux\,Multiplier \Rightarrow Flux\,Multiplier = \frac{Power\,Level \times \nu}{Q_{value}} \quad .$$

MCNPX calculates the system-averaged ν and Q value. The power level used for the flux multiplier calculation is the power entered on the *POWER* flag. The Q value used in the calculation is considered to be the prompt recoverable energy per fission event. Therefore, within the Q value, delayed gamma and beta heating contributions from the radioactive fission products are not considered. Nor within the Q value are delayed (n,gamma) capture reactions considered.

Consequently, the Q value is underestimated. Underestimating the Q value leads to an overestimation of the system fluxes and thus, an overestimation of the system collision densities. Because the equation for nuclide depletion is highly dependent on the collision densities:

$$\frac{dN(r,t)}{dt} \approx -\sum_{i}^{E} \phi_i(r,t)\Sigma_i(r,t)N_i(r,t) \quad .$$

Increasing the collision density leads to an overestimation of the material burnup. In the current depletion capability, three methods are used to correct this overestimation:

1. adjusting the Q value multiplier (B1 value on the *BOPT* flag; default = 1.0),
2. modifying the total thermal system recoverable energy by adjusting the power level entered on the *POWER* flag, and
3. altering the system power on the *PFRAC* flag.

2.1.7. Burn Materials

The materials to be burned must be listed on the *MAT* flag. Each "Mi" entry corresponds to the material number listed in Data Cards section of the input deck.

For example:

```
…
      BURN TIME=100,70
       MAT=1,3,4
       POWER=1.0
       PFRAC=1.0,1.0
       BOPT=1.0 -12 1.0
      C Material Cards
      m1
       8016.60c 4.5854e-2
       92235.60c 1.4456e-4
       92238.60c 1.9939e-2
       94238.60c 1.1467e-4
       94239.60c 1.0285e-3
       94240.60c 7.9657e-4
       94241.60c 3.3997e-4
       94242.60c 5.6388e-4
      m2 2004 -1.0
      m3 40000.60c -1.0
      m4 1001.60c 4.7716e-2
       8016.60c 2.3858e-2
       5010.60c 3.6346e-6
       5011.60c 1.6226e-5
      mt4 lwtr.01t
…
```

In this example, materials m1, m3, and m4 will be burned.

Burnup is calculated for the entire system, as well as for each individual material containing a fissile actinide. The total system burnup, as well as other important time-dependent parameters, is listed on the burn table.

For example:

neutronics and burnup data

step	duration (days)	time (days)	power (MW)	keff	flux	ave. nu	ave. q	burnup (GWd/MTU)
0	0.000E+00	0.000E+00	1.000E+00	1.15793	4.428E+15	2.878	209.106	0.000E+00
1	1.000E+02	1.000E+02	1.000E+00	1.00865	5.157E+15	2.900	209.094	5.892E+01
2	7.000E+01	1.700E+02	1.000E+00	0.98152	5.465E+15	2.920	208.965	1.002E+02...

For each individual material, another burn table is created that lists the fraction of fission power created by that specific material, as well as the individual burnup of that material. The power fraction is calculated for an individual material using the following methodology:

1. Determine if the material contains an actinide.
2. If yes, sum up the continuous energy fission energy created to obtain an individual burn material fission energy.
3. Sum up all of the total material fission energy contributions for each material that contains an actinide.
4. Calculate the power fraction as

$$power\ fraction = \frac{\left(\Phi\Sigma_f VQ\right)_i}{\sum_i \left(\Phi\Sigma_f VQ\right)_i} \quad .$$

The burnup for each individual material then is calculated using

$$Burnup = Burnup_{previous\ step} + \frac{Power\ Level \times Power\ Fraction \times Time \times PFRAC}{MTU} \quad .$$

[MTU = MTHM (metric tonnes of heavy metal) and is explained further in Section 2.1.8.]

When the burnup for each individual actinide is listed in the output, the material numbers for each individually burned material correspond to the incremental material order of the burned materials and not to the actual material number from the Data Cards section.

For example (corresponding to the BURN and Material Cards listed above):
…
Individual Material Burnup

Material #: 1

step	duration (days)	time (days)	power fraction	burnup (GWd/MTU)
0	0.000E+00	0.000E+00	1.000E+00	0.000E+00
1	1.000E+02	1.000E+02	1.000E+00	5.892E+01
2	7.000E+01	1.700E+02	1.000E+00	1.002E+02

Material #: 3

step	duration (days)	time (days)	power fraction	burnup (GWd/MTU)
0	0.000E+00	0.000E+00	0.000E+00	0.000E+00
1	1.000E+02	1.000E+02	0.000E+00	0.000E+00
2	7.000E+01	1.700E+02	0.000E+00	0.000E+00

Material #: 4

step	duration (days)	time (days)	power fraction	burnup (GWd/MTU)
0	0.000E+00	0.000E+00	0.000E+00	0.000E+00
1	1.000E+02	1.000E+02	0.000E+00	0.000E+00
2	7.000E+01	1.700E+02	0.000E+00	0.000E+00

…

In this example, materials 1, 3, and 4 were burned, and only material 1 contained fissionable actinides. The stated power fraction for material 1 is 1.000E+00 because material 1 supplied all of the fission power to the system.

2.1.8. Automatic Fission Yield Selection Process

The CINDER90 code offers a thermal, fast, high-energy fission yield for each fissile isotope contained in the CINDER.dat library file. The proper fission yield to be used for a specified problem is dependent on the impinging neutron energy at the interaction site. Because CINDER90 is a deterministic code that uses one-group constants and does not account for multi-energy behavior, knowledge of the neutron spectrum must be imported from the steady-state continuous energy calculation.

MCNPX determines which fission yield to use for a specified problem by calculating the integral fission rate for the defined energy boundaries (thermal, fast, and high energy), determining which energy range contains the majority of fissions, and then selecting the appropriate fission yield corresponding to the energy range containing the majority of fissions at each time step.

This calculation is completed separately for each burn material. Therefore, if a specific calculation warrants a thermal fission yield for one burn material and a fast fission yield for another burn material, MCNPX will be able to implement a thermal fission yield for the burn material experiencing a thermal spectrum and a fast fission yield for the burn material

experiencing a fast spectrum. The process is automatic; thus, users do not have to worry about selecting an appropriate fission yield that best represents their system because MCNPX will determine the correct fission yield automatically.

2.1.9. Metric Tonnes of Uranium (MTU)

MCNPX lists burnup in units of GWD/MTU. The MTU term calculated in MCNPX is actually the sum of the masses of isotopes containing >90 protons. Therefore, thorium and plutonium contribute to the MTU calculation. It is possible for elements containing >82 protons to fission; however, the probability of fission is very low. If a fuel ($82 < Z < 90$) is analyzed, the burnup must be adjusted to reflect appropriately the nature of how the burnup calculation is completed.

2.1.10. Isotope Reactivity Options

The *OMIT* flag allows the user to run a transport calculation without including the transport data from a specified isotope. This flag presents the user with the ability to investigate the reactivity effects that a certain isotope has on the analyzed system.

The *OMIT* flag has the following format: OMIT=J1,N1,I11,I12,...,J2,N2,I21,I22,...

Ji = ith material for which to omit nuclides Ii1, Ii2, etc.
If J1 = -1, then the omitted nuclide list is applied to all materials and J2, J3, etc., are not allowed. No default.

Ni = number of omitted nuclides listed for the ith material. No default.

Ii1, Ii2, … = 1st, 2nd, etc., omitted nuclide for the ith material. No default.

The *AFMIN* flag allows the user to determine below which mass fraction an isotope will be dropped from the transport calculation. The *A* value of *AFMIN* flag signifies the minimum atom fraction for all isotopes in which isotopes below that atom fraction will have their atom fraction set to zero. The default is 1.0E-10.

2.1.11. Models Option

The B3 section of the *BOPT* flag invokes the models option. Cross-section models are a heritage of the high-energy physics capabilities of MCNPX. The models are benchmarked for a variety of problems for neutron energies >150 MeV. The B3 section of the *BOPT* flag allows the user to disallow the use of models if the cross-section energy of interest is below the benchmarked value.

For the B3 section of the *BOPT* flag, the following options exist:

B3 = -1 Fatal error if models are used in the problem.

B3 = 0 Zeros out the atom fraction of any data using a model. This option runs only if the number of isotopes needed to be zeroed out does not exceed 100. It is preferable to determine which isotopes are needed to be zeroed out and to place them on the omit card for the burned material; however, this option exists as a simpler alternative to the omit card.

B3 = 1 Runs with models.

2.1.12. Fission Product Tracking/Output Frequency

The B2 value on the *BOPT* flag corresponds to the selected fission products used in the MCNPX transport process, as well as the format for the nuclide concentrations in the output file. MCNPX reports nuclide concentrations only for actinides listed on the material cards or generated by the isotope generator algorithm, as well as fission products listed on the material cards or generated by the isotope generator algorithm. If a material listed on a material card that does not correspond to one of the ZA numbers (where Z is the atomic number and A is the atomic mass) listed in the fission product array or the material is not an actinide (Z > 90), then the isotope is used in MCNPX transport but is not reported in the nuclide concentration section of the output file.

B2 = burn table output frequency, ordering, and content flag.

Input Value	Output Inventory Ordering
1 (default)	High to low, based on mass
2	High to low, based on activity
3	High to low, based on specific activity
4	Increasing zaid

Positive input values cause the output to be printed to the output file only at end of an entire job. Negative input values cause output at the end of each burn step.

Three tiers of fission-product content are available. Each tier corresponds only to those isotopes that are used for particle transport in MCNPX and the nuclide densities, which are reported in the output file. To select a specific tier, add zero (default), 10, or 20 to the magnitude of the B2 Input Value.

TIER	Fission-Product Content
1 (default)	Zr-93,Mo-95,Tc-99m,Ru-101,Xe-131,Xe-134, Cs-133,Cs-137,Ba-138,Pr-141,Nd-143,Nd-145.
2	All Incident Neutron Cross Sections contained in Fp Array included in current (v250) XSDIR
3	All isotopes contained in Fp Array

The fission product array:

01003,05010,05011,32072,32073,32074,32076,33075,34077,34079,34080,34082,35081,
36082,36083,36084,36085,36086,37085,37086,37087,38086,38088,38089,38090,39089,
39090,39091,40090,40091,40092,40093,40094,40095,40096,41095,41097,42095,42096,
42097,42098,42099,42100,43099,44100,44101,44102,44103,44104,44105,44106,45103,
45105,46104,46105,46106,46107,46108,46110,47109,47111,48110,48111,48112,48113,
48114,48116,49115,50116,50117,50118,50119,50120,50122,50123,50124,50125,50126,
51121,51123,51124,51125,51126,52122,52124,52125,52126,52128,52130,52132,53127,
53129,53130,53131,53132,53133,53134,53135,54128,54129,54130,54131,54132,54133,
54134,54135,54136,55133,55134,55135,55136,55137,56134,56136,56137,56138,56140,
57139,57140,58140,58141,58142,58143,58144,59141,59142,59143,59145,60142,60143,

60144,60145,60146,60147,60148,60150,61147,61148,61149,61151,62147,62148,62149,
62150,62151,62152,62153,62154,63151,63152,63153,63154,63155,63156,63157,64152,
64154,64155,64156,64157,64158,64160,65159,65160,66160,66161,66162

For example:

BOPT 1.0 -14 1.0 .

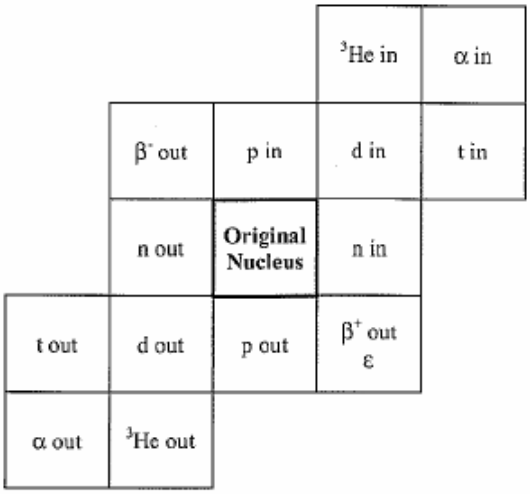
In this case, the fission product and actinide concentrations, as well as the burn tables, are listed at the end of each time step in increasing zaid order; the Tier-2 fission products are used in MCNPX transport and are listed in the output file as

- = list at the end of each time step,
4 = list isotope concentrations in increasing zaid, and
4 + 20 = use Tier-2 fission products.

2.1.13. The Isotope Generator Algorithm

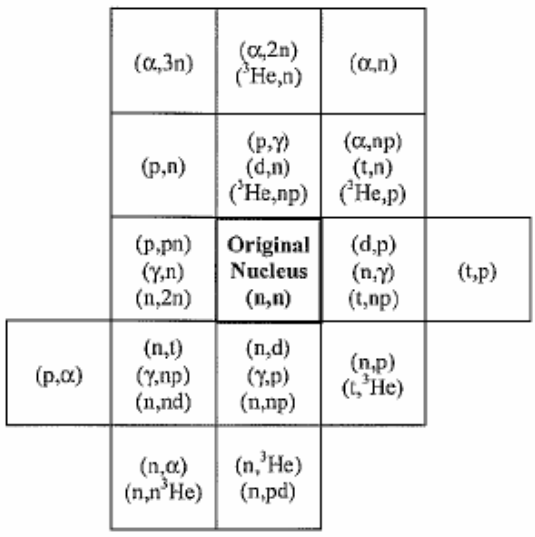
Capturing every decay chain product, from every initial parent isotope, for transport in MCNPX would be a very memory-intensive process. Also, although CINDER90 tracks decay and depletion cross-section data for 3456 isotopes, many of these isotopes do not contain useful transport information for MCNPX. To save computation time and reduce the influx of unimportant information, if an isotope is specified on an MCNPX material, only the immediate daughter products are tracked in MCNPX for particle transport. CINDER90 still tracks all of the daughter/granddaughter/great-granddaughter/etc., decay reactions for 3456 isotopes; therefore, the total isotopics listed in MCNPX are the true concentrations from the depletion process. However, the steady-state particle transport model includes only those isotopes listed on the material cards that are selected from the fission product array and produced by the isotope generator algorithm.

The following chart displays the isotopes generated for an isotope that has a $Z > 4$. The location of each generated isotope corresponds to the position of that isotope as it would appear in the Chart of the Nuclides:



n = neutron α = alpha particle
p = proton β^- = beta minus (negative electron)
d = deuteron β^+ = beta plus (positron)
t = triton ε = electron capture

Relative Locations of the Products of Various Nuclear Processes on the Chart of the Nuclides.



Changes Produced by Various Nuclear Reactions.

2.1.14. Proper Tracking of Entire Decay Chains

Because the isotope generator algorithm captures only the daughter reactions of the isotopes specified on the material card, the entire isotope decay chain will not be implemented into the MCNPX transport model and subsequently will not be tracked in the MCNPX output file. Understanding nuclide buildup and depletion is never a straightforward process; therefore, receiving nuclide concentrations of members of an isotopes decay chain may give insight into the

variation in isotope buildup and depletion. Further, decay chain members may have significant cross sections that would lead to altered MCNPX flux and collision density calculations.

For MCNPX to track a decay chain member, that isotope must be listed on the material card at beginning of life (BOL). Because the decay chain members will not be present at BOL, the decay chain member's zaid on the corresponding burn material card, with an atom density of 1E-36, can be input. Therefore, the buildup of that specific decay chain member will be tracked in the MCNPX transport calculation and the corresponding nuclide mass will be listed in the output file.

2.1.15. Example INPUT

The following example explains the input setup for the burn card:

```
BURN TIME=15.0,30.0,30.0 MAT=3,4 POWER=2.0
     OMIT=3,3,8017,92234,92239,4,1,92234
     BOPT=1.0 -11
```

This card specifies a power level of 2 MW, with time steps of 15 days, 30 days, and 30 days, for a total of 75 days. Materials 3 and 4 are included in the burn with isotopes 8017, 92234, and 92239 excluded from material 3 and isotope 92234 excluded from material 4. Output will be produced at the end of each burn step and ordered by decreasing mass, and Tier-2 fission products will be treated.

To avoid averaging (fluxes, densities, etc.) across multiple cells that share a material number, a unique material for each cell of interest can be provided.

Print Tables 40 and 50 are repeated in the output file for each time step, giving the updated atom fractions and densities. Print Table 55 provides the burnup results at the end of each time step.

2.2. CEM03 Upgrade

The CEM2K physics package has been replaced with the new CEM03 physics package[1] and will soon also have the new LAQGSM physics package. The MCNPX user interface has not changed: if the 9th entry on the LCA card is 1, then CEM03 will be used.

CEM03.01[2] is the latest modification of the improved Cascade-Exciton model (CEM). It is a completely new, updated, and modified version, not just an incremental improvement, in comparison with its predecessors, CEM2k+GEM2,[1,2] CEM2k,[3] CEM98,[4] CEM97,[5] and CEM95.[6]

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[1] S. G. Mashnik, K. K. Gudima, M. I. Baznat, A. J. Sierk, R. E. Prael, and N. V. Mokhov, "CEM03.S1, CEM03.G1, LAQGSM03.S1, and LAQGSM03.G1 Versions of CEM03.01 and LAQGSM03.01 Event-Generators," Los Alamos National Laboratory report LA-UR-06-1764 (March 6, 2006), also available at http://mcnpx.lanl.gov > documents.

[2] Stepan G. Mashnik, Konstantin K. Gudima, Arnold J. Sierk, Mircea I. Baznat, and Nikolai V. Mokhov, "CEM03.01 User Manual," Los Alamos National Laboratory report LA-UR-05-7321 (2005); RSICC Code Package PSR-532, http://www-rsicc.ornl.gov/codes/psr/psr5/psr-532.html/ (2006).

CEM03.01 describes reactions induced by nucleons, pions, and photons as a three-stage process: IntraNuclear Cascade (INC), followed by preequilibrium emission of particles during the deexcitation of the excited residual nuclei formed during the INC, followed by evaporation of particles from or fission of the compound nuclei. If the excited residual nucleus produced after the INC has a mass number A < 13, CEM03.01 uses a recently updated and improved version of the Fermi Breakup model to calculate its decay instead of considering a preequilibrium stage followed by evaporation from compound nuclei. CEM03.01 considers also coalescence of complex particles up to ^{4}He from energetic nucleons emitted during the INC.

The main improvements of CEM03.01 in comparison with its predecessors are

2.2.1. Intra Nuclear Cascade (INC)

We developed new approximations to describe more accurately experimental elementary energy and angular distributions of secondary particles from hadron-hadron and photon-hadron interactions using available data and approximations published by other authors. We have normalized photonuclear reactions to detailed systematics developed by others.[78] The condition

[1] S. G. Mashnik, K. K. Gudima, and A. J. Sierk, "Merging the CEM2k and LAQGSM Codes with GEM2 to Describe Fission and Light-Fragment Production," Los Alamos National Laboratory report LA-UR-03-2261 (2003); E-print: nucl-th/0304012; Proc. 6th Int. Workshop on Shielding Aspects of Accelerators, Targets and Irradiation Facilities (SATIF-6), April 10–12, 2002, Stanford Linear Accelerator Center, CA 94025, USA, NEA/OECD, Paris, France, 2004, pp. 337–366.

[2] Stepan G. Mashnik, Arnold J. Sierk, and Konstantin K. Gudima, "Complex Particle and Light Fragment Emission in the Cascade-Exciton Model of Nuclear Reactions," Los Alamos National Laboratory report LA-UR-02-5185 (2002); E-print nucl-th/0208048.

[3] S. G. Mashnik and A. J. Sierk, "CEM2k—Recent Developments in CEM," Los Alamos National Laboratory report LA-UR-00-5437 (2000); Proc. of the 2000 ANS/ENS Int. Meeting, Embedded Topical Meeting Nuclear Applications of Accelerator Technology (AccApp00), November 12–16, 2000, Washington, DC (USA), American Nuclear Society, La Grange Park, IL, 2001, pp. 328–341; E-print: nucl-th/0011064.

[4] A. V. Prokofiev, S. G. Mashnik, and A.J. Sierk. "Cascade-Exciton Model Analysis of Nucleon-Induced Fission Cross Sections of Lead and Bismuth at Energies from 45 to 500 MeV," Los Alamos National Laboratory report LA-UR-98-0418 (1998); E-print: nucl-th/9802027; *Nucl. Sci. Eng.* (1999), Vol. 131, No. 1, pp. 78–95.

[5] S. G. Mashnik and A. J. Sierk, "Improved Cascade-Exciton Model of Nuclear Reactions," Los Alamos National Laboratory report LA-UR-98-5999 (1998); E-print: nucl-th/9812069; Proc. Forth Int. Workshop on Simulating Accelerator Radiation Environments (SARE-4), Knoxville, TN, September 13–16, 1998, Oak Ridge National Laboratory, 1999, pp. 29–51.

[6] S. G. Mashnik, "User Manual for the Code CEM95," Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, Dubna, Russia (1995), CEM95 Code Package IAEA1247 distributed by the OECD Nuclear Energy Agency, Paris, France, 1995, http://www.nea.fr/abs/html/iaea1247.html.

[7] S. G. Mashnik, K. K. Gudima, M. I. Baznat, A. J. Sierk, R. E. Prael, and N. V. Mokhov, "CEM03.01 and LAQGSM03.01 Versions of the Improved Cascade-Exciton Model (CEM) and Los Alamos Quark-Gluon String Model (LAQGSM) Codes," Los Alamos National Laboratory Research Note X-5-RN (U) 05-11; Los Alamos National Laboratory report LA-UR-05-2686 (2005).

[8] S. G. Mashnik, M. I. Baznat, K. K. Gudima, A. J. Sierk, and R. E. Prael, "CEM03 and LAQGSM03: Extension of the CEM2k+GEM2 and LAQGSM Codes to Describe Photo-Nuclear Reactions at Intermediate Energies (30 MeV to 1.5 GeV)," E-print: nucl-th/0503061, *J. Nucl. and Radiochem. Sci.*, Vol. 6, No. 2, pp. A1–A19 (2005).

for transition from the INC stage of a reaction to preequilibrium was changed; on the whole, the INC stage in CEM03.01 is longer, whereas the preequilibrium stage is shorter in comparison with previous versions. The algorithms of many INC routines were changed, and almost all INC routines were rewritten, which sped up the code significantly; some preexisting bugs in the INC were fixed.

2.2.2. Preequilibrium (PREC)

The condition for transition from the preequilibrium stage of a reaction to evaporation/fission was changed; on the whole, the preequilibrium stage in CEM03.01 is shorter, whereas the evaporation stage is longer in comparison with previous versions. The widths for complex-particle emission were changed by fitting the probability of several excitons to "coalesce" into a complex particle that may be emitted during the preequilibrium stage to available experimental data on reactions induced by protons and neutrons.[1] Algorithms of many PREC routines were changed, and almost all PREC routines were rewritten, which sped up the code significantly; some bugs were discovered and fixed.

2.2.3. Evaporation and/or Fission

The evaporation and fission stages of reactions are calculated by CEM03.01, with an updated and improved version of the Generalized Evaporation model code GEM2[2] by Furihata, which considers evaporation of up to 66 types of different particles and light fragments (up to ^{28}Mg). In comparison with GEM2, the calculation of fission widths in CEM03.01 was changed by fitting the ratio of the level-density parameters at the saddle point to that in the evaporation channel to the systematics of proton-induced fission cross sections by Prokofiev.[3,4] Several routines by Furihata from GEM2 were slightly modified in CEM03.01; some bugs found in GEM2 were fixed.

2.2.4. Coalescence

The coalescence model implemented in CEM is described is improved.[5] In comparison with its initial version, we have changed the coalescence momentum radii p_0 for the various light composite particles up to ^{4}He by fitting them to measured data on nucleon-induced reactions at energies up to 1 GeV.

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[1] S. G. Mashnik, M. I. Baznat, K. K. Gudima, A. J. Sierk, "CEM03.01 and LAQGSM03.01 Improvement for Gas-Production Cross Section Calculations," Los Alamos National Laboratory report LA-UR-05-8447 (2005); Proc. 14th Biennial Meeting on the Radiation Protection and Shielding Division, Carlsbad, New Mexico, USA, April 3–6, 2006, CD with the RPSD2006 Procs., ANS, La Grange Park, IL, USA, 2006, ISBN: 0-89448-693-4, pp. 169–172.

[2] S. Furihata, "Statistical Analysis of Light Fragment Production from Medium Energy Proton-Induced Reactions,'" Nucl. Instrum. Methods B 171 (2000) 252–258; PhD thesis, Tohoku University, March, 2003 (and references therein).

[3] A. V. Prokofiev, "Compilation and Systematics of Proton-Induced Fission Cross-Section Data," NIM, A463 (2001) 557–575.

[4] A. V. Prokofiev, S. G. Mashnik, and W. B. Wilson, "Systematics of Proton-Induced Fission Cross Sections for Intermediate Energy Applications," Los Alamos National Laboratory report LA-UR-02-5837 (2002), E-print: nucl-th/0210071.

[5] V.D. Toneev, K.K. Gudima, "Particle Emission in Light and Heavy-Ion Reactions," *Nucl. Phys.* A400 (1983) 173c–190c.

2.2.5. Fermi Breakup

The Fermi Breakup model used in CEM is improved.[1,2] In comparison with its initial version, we have modified the model to decay some unstable light fragments that could be produced by the original Fermi Breakup model. Several bugs observed in the original version were fixed.

2.2.6. Additional Notes

Almost all routines of CEM03.01 were rewritten and many algorithms were changed so that the code is much faster now than all its predecessors. The output of CEM03.01 was significantly extended, which allows us to calculate with the standard CEM03.01 many more different characteristics of nuclear reactions, in comparison with its predecessors.

CEM03 is more accurate but somewhat slower than the CEM2K it replaces. CEM problems no longer track. Problems using model physics and having photonuclear reactions also no longer track.

2.3. Long File Names

MCNPX file names may now be 40 characters long. The execute line message may now be 240 characters long. File names also may be paths.

For example:

MCNPX *name* = ..\..*destination_output_files.* *inp* = ..*input_file* .

In this example, the input file is named *input_file* and is located in the next directory up.

MDATA Files

Mesh tally MDATA files now use the *name* option. In the above example, the MDATA file would be named *destination_output_files.d* and would be put in the directory ..\..\ .

Implementation Details

The 40-character length is set by the parameter *lfilen = 40* in *module_global_parameters, GLOBAL1_zc.F* . Thus, longer file names should be possible but have not been tested.

In some cases, warnings and fatal-error messages will give only the first eight characters of a file name because of format constraints. In most cases, the rewriting of all formats containing file names result in cleaner output. The full file name usually is allowed. Short file names no longer are followed by blanks to achieve the old eight-character file name length.

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[1] N. Amelin, "Physics and Algorithms of the Hadronic Monte-Carlo Event Generators. Notes for a Developer," CERN/IT/ASD Report CERN/IT/99/6, Geneva, Switzerland (1999).

[2] GEANT4, Users's Documents, Physics Reference Manual," December 8, 1998, http://wwwinfo.cern.ch/asd/geant4/G4UsersDocuments/UsersGuides/PhysicsReferenceManual/html/PhysicsReferenceManual.html.

2.4. Terminate Tallies at Desired Precision

A new input card, "STOP", has been added to enable stopping of calculations when a desired tally precision is reached:

STOP NPS *n* CTME *m* F*k e* .

This card will cause MCNPX to stop after *n* histories, after *m* minutes, or when the tally fluctuation chart bin of tally *k* has a relative error less than *e*.

MCNPX will stop at the first met criteria.

For radiography problems, the second NPS card entry, *n*, may be provided to specify how many histories are used for direct radiography tally contributions:

STOP NPS *n m* .

For multitasking calculations, CTME will be checked only at rendezvous points, where all tasks rendezvous for tally fluctuations and other activities.

The tally precision stop will be checked only at rendezvous points for the tally bin of the tally fluctuation charts. Thus, the calculation usually will proceed for a short time after the desired error is achieved. Thus,

STOP F111 .05

will cause MCNPX to stop at the first rendezvous for which the relative error is less than 0.05. That is, MCNPX may stop at error = 0.048 or other value slightly less than 0.05.

3.0. MCNPX 2.6.B FEATURE EXTENSIONS AND ENHANCEMENTS

Several MCNPX features have been extended and have included changes or additions to the user interface:

- proton step-size control: HSTEP on M card (GWM),
- new photon emission data: PHTLIB (REP/GWM)
- new S(α,β) scattering law (REM/GWM/JSH),
- differential data tallies extended to table physics (GWM),
- separate printout of induced fission multiplicity (JSH),
- geometry plot basis vectors (GWM),
- removal of tracking fixes (JSH),
- extension of ZAID identifiers (GWM),
- LINLIN contour plot defaults (GWM), and
- additional enhancements.

3.1. Proton Step-Size Control

The proton step size can be controlled by a new keyword, *hstep*, on the material *Mn* card:

Mn hstep = m .

For example,

M123 estep = 10 hstep = 15 .

The *hstep* keyword for protons works just like the *estep* keyword for electrons. The *hstep* keyword causes the number of proton substeps per energy step to be increased to *m* (15 in the above example) for the material (123 in the above example). If *n* is smaller than the built-in default found for this material, the entry is ignored. Both the default value and the estep value actually used are printed in *Print Table 85* in the MCNPX output file.

The *estep* keyword is used only for electrons, and *hstep* is used for all other charged particles. If *estep* is specified and *hstep* is not, then the *estep* value is used for *hstep* to preserve backward compatibility.

3.2. New Photon Emission Data

The "new" Nov 2001 BCDLIB gamma emission data—which becomes PHTLIB in binary form—are now the default. The BCDLIB library contains a better description of the gamma decay process and produces a better gamma decay spectrum. Gamma emission from metastable states is blocked for half-lives >1 ms. Thus, MCNPX consistently provides the prompt emission spectra. The BCDLIB data contain the nuclear structure data needed to generate deexcitation photons.

The BCDLIB file is found in the MCNPX source directory under Data/LCS. When MCNPX is compiled, the PHTLIB (binary version) is created. The PHTLIB creation also has been corrected to eliminate several long-lived decay gammas that were >1 ms.

Users of executable MCNPX versions should use the latest PHTLIB file. After unzipping Win32.zip or Linux.tar.gz, etc., the files PHTLIB and BERTIN in the data directory should be used and put in with the other cross sections from ENDF, etc.

Users who compile MCNPX should get the latest PHTLIB from their build directory,

Build_directory/src/phtlib/phtlib .

3.3. New S(α,β) Scattering Law

A new S(α,β) tabular data-scattering law from NJOY (REM, T-16) was added for compatibility with forthcoming ENDF/B-VII data libraries.

3.4. Differential Data Tallies Extended to Table Physics

Differential cross-section data now may be calculated and tallied in the table physics region. When *noact = -2* (8th entry on the *LCA* card), the sourced particle immediately collides in the source material. All subsequent daughter particles then are transported without further collision, as if in a vacuum. Differential cross sections (secondary energy and/or angle distributions, residual nuclei and light ions, and other information) then can be calculated and tallied with an F1 or F8 tally. The tallied data then can be plotted.

The *noact = -2* option no longer automatically sets all physics to model physics. Now, table physics is used whenever possible to get the differential data actually used in a given problem. To get the differential data with models only, the use of table data can be turned off with the *PHYS:pl* card, 5th entry.

.

3.5. Separate Printout of Induced Fission Multiplicity

Induced fission multiplicity now is printed separately instead of being combined with spontaneous fission in *Print Table 117*.

3.6. Geometry Plot Basis Vectors

MCNPX now forces the geometry plot coordinate system always to be right-handed. Previously, it was possible to specify left-handed coordinate systems in some cases, which led to plotting errors or easily misinterpreted plots.

3.7. Remove Tracking Fixes

The 20th entry on the *DBCN* now causes MCNPX26B to track MCNPX2.5.0 instead of MCNP4C3 and MCNPX2.4.0.

3.8. Interrupts in Electron Tracking

The <ctrl-c> interrupts now work during electron tracking. Normally, at the start of each <ctrl-c> particle track, or trajectory, MCNPX checks to see if the interrupt flag has been set. However, for electrons that may have many substeps, another tracking algorithm, DBMIN, has interrupts that previously were not checked. DBMIN finds the minimum distance to a boundary from a point, and then all tracking (substeps) within that distance of the point does not have to check bounding surfaces. By checking for <ctrl-c> interrupts in DBMIN, these interrupts now work better for electron problems (GWM, 4/19/06).

3.9. Extended ZAID Identifiers

The ZAID identifier may now be alphanumeric to allow more nuclides. Examples would be 1001.abc or 1001.xyc or 1001.a9c, all of which are continuous-energy neutron libraries.

3.10. LINLIN Contour Plot Default

The default interpolation scheme for tally contour plots (*FREE SC*) is now LINLIN to avoid carrying over a default of LINLOG, LOGLIN, or LOGLOG, which then truncates out all the values less than zero. This extension was suggested by Róbert Kákonyi at the University of Szeged, Hungary.

3.11. Weight Window Contour Plot Coloring

The weight window contour plots now plot white instead of blue for zero (no window game played) and negative (zero importance) windows instead of blue for zero windows (GWM 4/3/06).

3.12. Deleted Segmenting Surfaces

The tally segmenting capability (FSn tally card) was extended to work for segmenting surfaces that are deleted duplicate surfaces. The undeleted duplicate surface then is used automatically. This enhancement was suggested by Jeff Bull (Franz X. Gallmeier/GWM, 4/24/06).

4.0. MCNPX 2.6.B CORRECTIONS

4.1. Significant Problem Corrections

The following problems could cause incorrect answers. Fortunately, they occur only in very special situations and affect only a few MCNPX users.

4.1.1. Auger Electrons below Energy Cutoff

Auger electrons were not made from photoelectric fluorescence, and tally heating from fluorescence was neglected when produced by photons below the photon energy cutoff. The effect is small and has been found in all previous MCNP and MCNPX versions. The affected tallies are the MCNPX +F6 and F6:e tallies. A $2 award was made to Greg Cunningham (ISR-1, LANL) (D-5:JSH-2006-18) (GWM).

4.1.2. Detectors in Lattice Geometries

Point detectors in lattice geometries could cause a crash. Possibly answers could be wrong without a crash. The error results because the *levp* variable could be changed erroneously in (and thus needed to be restored after) the do 695 loop in subroutine *tallyd*. The possible problem has occurred in all previous MCNP and MCNPX versions. A $2 award was made to Kin Yip (Brookhaven National Laboratory) (D-5:JSH-2006-111) (GWM, 3/7/06).

4.1.3. KCODE/PRDMP 5th Entry

If the PRDMP 5th entry is not one for KCODE problems, then RUNTPE files and other problems can occur because an array overflows. The problem occurs only if the TFC update frequency, NPD, the 5th entry, is larger than the current KCODE cycle, KCY, when adding to the tally fluctuation charts. In most cases, this is not a problem because the default value for NPD with KCODE is "1". A €20 award was made to Sergey Belousov (INRNE-BAS, Sophia, Bulgaria) (D-5:JSH-2006-112) (GWM 4/19/06).

4.1.4. Universe Map Crash

The universe map for lattice/repeated structures geometries, Print Table 128, could occasionally have an array overflow that caused a crash in rare cases, thus affecting all previous code versions. A $2 award was made to Benjamin Amiri, LANL, D-5 (D-5:JSH-2006-142) (GWM 5/26/06).

4.2. Minor Problem Corrections

The following problems do not cause wrong answers, but they may cause crashes when encountered. In any case, they occur only in very special situations and affect only a few MCNPX users.

4.2.1. Cylindrical Weight Window Mesh

Neither the weight window nor the weight-window generator cylindrical meshes properly used the theta bin. The improper use affected using, generating, and plotting these weight-window meshes. Cylindrically symmetric meshes (no theta bins) were unaffected. Answers also were not affected because variance reduction affects only efficiency (GWM/JSH).

4.2.2. I8 Mesh Tally Plots

Improper initialization caused mesh tallies not to plot in MCNPX versions compiled with the I8 configuration option, namely, 64-bit integer code versions. A $20 award was made to Bill Schmitt (Draper Labs, Massachusetts) (D-5:JSH-2005-190) (GWM/JSH).

4.2.3. Continue Cards for Input with FATAL Errors

Continue cards failed for input with FATAL errors. A $2 award was made to Valery Taranenko (GSF, Germany) (D-5:JSH-2005-191).

4.2.4. Sometimes Can Plot Only First Mesh Tally

Geometry plots in the command mode (the mode with the PLOT> prompt) for mesh tallies failed in some cases:

```
PLOT> TALnn.m   .
```

The above command would plot only the first mesh tally if there were non-mesh tallies in the same problem (JSH).

4.2.5. Incorrect KCODE/Message Passing Interface (MPI) Error Message

The warning error message, "KCODE with load balancing is very inefficient.", had a bad format that caused a crash whenever criticality problems were run in parallel with load balancing. A €20 award was made to Steven van der Marck (NRG, Petten, Netherlands) (D-5:JSH-2005-239) (GWM).

4.2.6. Incorrect LCS Error Message

The LAHET (LCS) diagnostic message for "projectile negatives" and "target negatives" incorrectly listed the atomic number twice rather than the Z-number and then the atomic number. A $2 award was made to Igor Remec (ORNL) (D-5:JSH-2005-238) (GWM).

4.2.7. Mesh Tally Writing to Backup runtpe

The mesh tallies could cause a crash when writing to backup *runtpe* files. The backup *runtpe* files are those temporarily created for the *PRDMP 3J N* option, which allows overwriting the *runtpe* file with only the last *N* dumps to conserve space. A €20 award was made to Steven Van der Marck (NRG, Netherlands) (D-5:JSH-2006-005), who also provided the correction.

4.2.8. Pulse-Height-Tally Variance Reduction Techniques with MPI

Pulse-height tallies (F8) with variance reduction techniques crashed when run in parallel with MPI. A $20 award was made to Ronald McConn (PNL) (D-5:JSH-2006-019) (GWM).

4.2.9. PTRAC and Event Log Omission

Both PTRAC (PTRAC card) and Event Logs (DBCN card) write the individual events of a history. Neither wrote collisions using physics models (rather than data tables) in the mix-and-match energy range. (GWM, 4/12/06)

4.2.10. FM Tally Multiplier in Model Physics Regime

The FM (tally multiplier) multiplies tallies by cross sections and other quantities from the MCNPX data libraries. If the tally is at an energy above the highest energy in the data tables, that is, in the model physics energy region, then MCNPX (like MCNP) uses the cross section at the highest energy of the table. However, when a model is used instead of a data table, then no data table values are available at lower energies and MCNPX may crash or get erroneous answers. In some cases, this crash happens in the mix/match energy region between the lowest data table energy and the highest data table energy. The new approach (starting with MCNPX 26B) is to issue an error message at the first occurrence of an FM multiplier above the energy range of a data table and then to return a zero multiplier (Michael R. James, 4/18/06).

4.2.11. Make Clean Enabled for PC Build

The Make Clean command now works at all levels of the build system on PCs (GWM, 5/25/05).

4.2.12. Zero Electron Mesh Tallies

Electron mesh tallies gave all zeroes in void regions. Corrected by GWM, 2/23/06, and $2 awarded to Carlo Petrovich (ENEA, Bologna, Italy) (D-5:JSH-2006-101, 4/24/06).

Note that a low-density issue also exists in the workaround, namely adding materials of very low densities. For heavier-charged particles, a numerical problem occurs in the straggling routines with densities <~1e-9 g/cm^3 and with densities <~1e-15 g/cm^3 for electrons. For now, users should avoid such low densities.

5.0. FUTURE WORK

The following projects are at least partially funded and are actively being developed. These capabilities should be available soon in a future MCNPX version:

- additional Cinder90 capabilities
  - delayed neutrons physics models;

  - delayed gamma physics models, and
  - fixed-source depletion.
- Spherical geometries for superimposed weight window mesh and weight window generator
- improved convergence of eigenfunctions in criticality problems
- improved physics with the LAQGSM/CEM03 model
- integration of HTAPE tallies directly into MCNPX, including continue runs
- heavy-ion tracking and interactions
- electric and magnetic field tracking

The following projects are on our wish list. Some have been partially developed but await further funding.

- detectors and DXTRAN for all neutral particles at all energy ranges with anisotropic scattering (currently approximated as isotropic for models),
- CAD link,
- secondary particle angle biasing for isotropic distributions,
- neutral particle perturbation techniques extended to physics model region,
- plotting of physics model total and absorption cross sections, and
- forced collisions for neutral particles extended to physics models.